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Hybrid Particle-Continuum Methods for Nonequilibrium Gas and Plasma Flows

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Abstract. Two different hybrid particle-continuum methods are described for simulation of nonequilibrium gas and plasma dynamics. The first technique, used for nonequilibrium hypersonic gas flows, uses either a continuum description or a particle method throughout a flow domain based on local conditions. This technique is successful in reproducing the results of full particle simulations at a small fraction of the cost. The second method uses a continuum model of the electrons combined with a particle description of the ions and atoms for simulating plasma jets. The physical accuracy of the method is assessed through comparisons with data measured in space. These examples illustrate that the multi-scale physical phenomena associated with nonequilibrium conditions can be simulated with physical accuracy and numerical efficiency using such hybrid approaches.

Keywords: hybrid methods, nonequilibrium gas dynamics, hypersonic flow, plasma propulsion
PACS: 47.45.-n; 47.70.Nd; 47.40.Ki; 52.65.Ww

INTRODUCTION

Nonequilibrium conditions occur in the gas and plasma flows of many real systems. One form of nonequilibrium concerns the generation of non-Maxwellian velocity distribution functions (VDFs). Physically, such nonequilibrium is produced by very strong gradients in flow field properties, for example ion shock waves and boundary layers, and by rarefied flow conditions. Another form of nonequilibrium concerns different species in the gas or plasma having very different VDFs from one another. In this article, a summary is provided of on-going development and application of two different hybrid fluid-particle methods for simulating these types of nonequilibrium flows. The first method combines solution of the Navier-Stokes equations using traditional methods from Computational Fluid Dynamics (CFD) with the particle-based direct simulation Monte Carlo (DSMC) technique [1]. This hybrid method decides, based on local flow conditions, whether to use CFD or DSMC in each region of a flow field. The DSMC technique is more physically accurate in strongly nonequilibrium regions, but is at least an order of magnitude slower than CFD. The performance of this method in terms of physical accuracy and numerical efficiency is illustrated through its application to hypersonic gas flows. The second hybrid method uses fluid and particle methods everywhere to simulate the plasma jets created by spacecraft propulsion systems [2]. In this technique, electrons are modeled using a fluid approach in which their conservation equations are solved using CFD methods. The heavy species (ions and atoms) are modeled using a combination of two particle methods. The DSMC technique is again employed to simulate collisions while the Particle In Cell (PIC) method is used to self-consistently accelerate ions in electro-static fields. The performance of this hybrid method is illustrated through its application to simulate plasma jets created by a spacecraft Hall thruster.

HYBRID METHOD FOR NONEQUILIBRIUM GAS FLOWS

For relatively low altitude portions of a hypersonic vehicle entry trajectory, the atmospheric density is relatively high, and simulations of flows around hypersonic vehicles should be performed using traditional Computational Fluid Dynamics (CFD) by solving either the Euler or the Navier-Stokes (NS) equations. At very

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high altitudes, at the edge of an atmosphere, the density is low such that there are very few collisions between the molecules and atoms in the flow around the vehicle. This rarefied flow regime can be computed using the direct simulation Monte Carlo (DSMC) method [3]. Relatively speaking, CFD methods for solving the NS equations are about an order of magnitude faster than the DSMC method. However, the lack of collisions in the low density gas makes the physics of the NS equations invalid.

A flow configuration that is characterized as being in the continuum regime overall can often contain localized regions of rarefied flow. Hypersonic flow over a cylinder provides an excellent example of this behavior, and the relevant phenomena are illustrated in Fig. 2. In such a flow, localized regions of rarefied flow may occur in: (1) the bow shock wave; (2) the boundary layer; and (3) the wake. In the cases of the bow shock and boundary layer, the local rarefaction is caused by the very strong gradients that produce small localized length scales that in turn produce large localized Knudsen numbers. In the wake, the density is a small fraction of that in the forebody flow and rarefaction is caused here directly by the associated large mean free path.

To compute such flows with existing computational tools we face the dilemma of either: (1) using CFD and accepting that there will be some (unknown) error associated with inaccurate physical modeling of the locally rarefied regions; or (2) trying to use the DSMC technique and accepting the incredibly high computational cost, especially for three dimensional flows. Thus, either CFD or DSMC on its own fails to provide a comprehensive computational modeling capability across all flow regimes encountered by a hypersonic vehicle. A natural solution to this problem is to develop a hybrid simulation technique that employs a CFD method for as much of the flow field as possible (due to its superior numerical performance) that switches to using DSMC only in those regions of the flow where the physics description provided by the CFD method is inadequate.

Continuum Computational Fluid Dynamics

Under continuum flow conditions, the traditional methods of Computational Fluid Dynamics (CFD) can be employed in which the basic conservation equations are solved numerically. LeMANS is a hypersonic CFD code that solves the 2D/3D Navier-Stokes equations using a line implicit method on general unstructured meshes. The code is parallelized using domain decomposition. Thermo-chemical non-equilibrium effects are included by solving a separate finite-rate vibrational energy equation, as well as individual species conservation equations that include source terms due to finite-rate chemistry. The ability to simulate a weakly ionized gas is included. Further details of the code can be found in [4].

The Particle-Based Direct Simulation Monte Carlo Method

The DSMC technique uses the motions and collisions of particles to perform a direct simulation of nonequilibrium gas dynamics [3]. A key step in DSMC is the separation of particle motion and collision. The particles are first moved through physical space by the product of their individual velocities and a time-step that is smaller than the local mean free time. After movement, the particle locations are fixed, the particles are collected into cells that have dimensions of the local mean free path, and in each of these cells a number of collisions is processed consistent with local flow conditions. Macroscopic flow properties such as density and temperature are obtained by time-averaging particle properties in the cells over several thousand iterations. The DSMC technique is the standard numerical method for simulating rarefied hypersonic flows.

MONACO is a parallel implementation of the DSMC method in which a computational cell is taken as the basic unit of the simulation [5]. Using the cell as the basic unit, rather than using the particle as in the usual DSMC algorithm, provides great flexibility in terms of using unstructured grids and parallel domain decomposition. MONACO contains models for a variety of physical phenomena including collisional momentum exchange, rotational energy exchange, vibrational energy exchange, chemical reactions, and wall collisions.

A Hybrid CFD-DSMC Method

A hybrid CFD-DSMC approach developed at the University of Michigan is called the Modular Particle Continuum (MPC) method [1] and merges existing CFD and DSMC codes. The accuracy of a hybrid particle-continuum method relies on the proper positioning of the DSMC-CFD interfaces. The interface must lie in near-equilibrium regions where solution of the NS equations will introduce minimal or no error. Typically, particle and continuum regions are determined by evaluating a continuum breakdown parameter in the flow field. The MPC method uses the gradient-length Knudsen number:

$$Kn_{GLL} = \frac{\lambda}{Q}\nabla Q \tag{1}$$

where Q represents local flow quantities such as density, temperature, or velocity magnitude, λ is the local mean-free-path, and the gradient is evaluated in all directions to determine the maximum gradient. It has been shown for hypersonic flows [6] that, in regions of the flow field where $Kn_{GLL} < 0.05$, the discrepancy between a NS and DSMC solution is less than 5%. Thus, these regions could be solved using a NS solver with little error. The MPC method begins with a NS solution of the entire flow field and then uses Eq. (1) to decompose the domain into CFD and DSMC regions.

The MPC method uses state-based coupling to transfer information between particle and continuum regions. After evaluation of the breakdown parameter, the particle region is extended by a few extra cells into the continuum domain to create an overlap region. The overlap regions help to improve accuracy of the DSMC fluxes. Next, one row of NS and two rows of DSMC boundary cells are initialized. The DSMC and NS domains are then coupled by transferring information across the interfaces. With state-based coupling, this involves updating the boundary conditions of each solver. In this way, information transfer into both the particle and continuum regions is handled through existing boundary procedures already used by both solvers. The DSMC boundary cells are continually filled with particles consistent with the flow properties in the corresponding NS cell using the Chapman-Enskog distribution based on the local macroscopic state and gradients, known from the NS solver. As particles in the DSMC domain interact and their distributions evolve in time, the MPC method also tracks the macroscopic variation in each DSMC cell. In order to provide these averaged properties with minimal statistical scatter, a mixture of spatial and temporal averaging is used. Specifically, MPC uses the sub-relaxation technique proposed by [7]. These averaged DSMC properties are then used to update boundary conditions for the NS solver.

Figures 1 illustrate the performance of the hybrid code for computation of normal shock waves of argon. Normalized density profiles for a Mach 9 shock are shown in Fig. 1(a). The CFD solution of the Navier-Stokes equations predicts a shock that is thinner than the experimental measurements of Alsmeyer [8] whereas DSMC provides almost perfect agreement. The hybrid code is initialized to the incorrect CFD result and "corrects" it such that it also provides excellent agreement with the measured data. Figure 1(b) demonstrates the very good agreement obtained with the hybrid method across a range of shock Mach numbers.

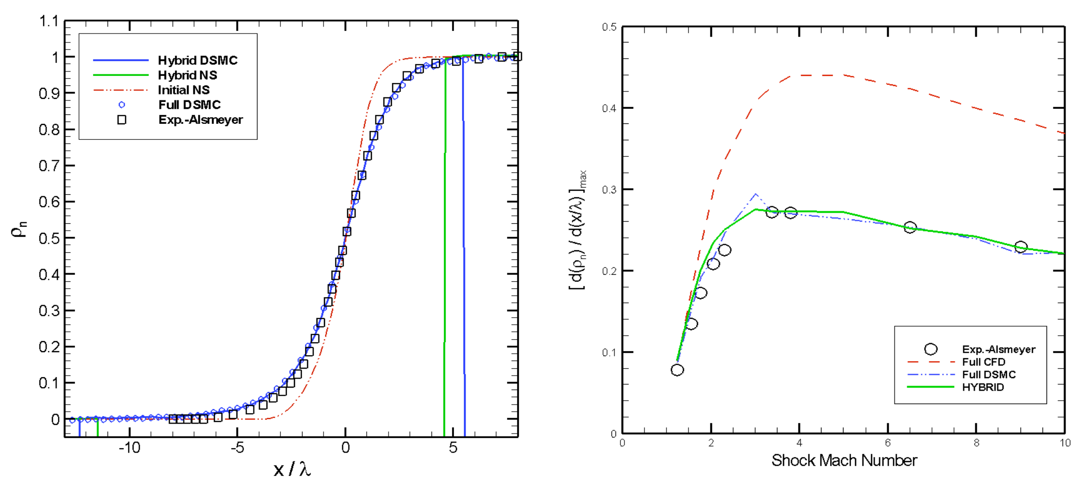

FIGURE 1. Argon shock waves: (a) normalized density profile at Mach 9; (b) reciprocal shock thickness.

Figures 2 illustrate the performance of the hybrid code for two dimensional, Mach 12 flow of nitrogen over a cylinder. In Fig. 2(a), significant differences for the temperature contours are found between the CFD (lower) and DSMC (upper) solutions. Again, the hybrid simulation is initialized to the (presumably) incorrect CFD result, and then modifies it to provide almost perfect agreement with the full DSMC computation. Indeed, as illustrated in Fig. 2(b), the level of agreement between solutions from full DSMC and the hybrid method agree at the level of the velocity distribution function. Significantly, in the best case we have found thus far for two-dimensional configurations, the hybrid code produces essentially the same solution as full DSMC at a factor of 30 lower overall computational cost while using one fifth of the amount of computer memory [9]. Current work is focused on extension of the hybrid method to 3D and further research will be required to extend the technique to simulation of chemical reactions.

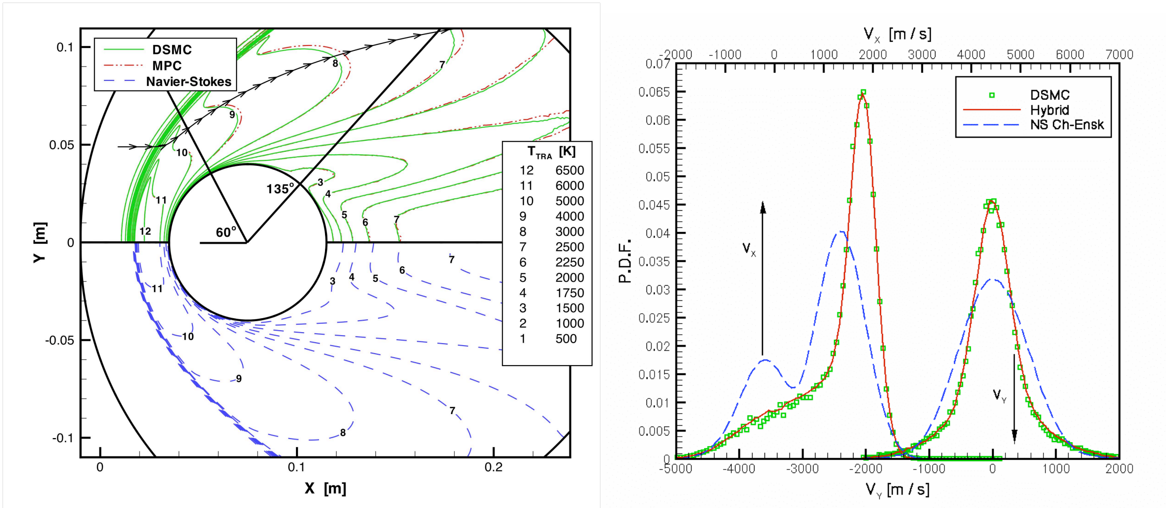

FIGURE 1. Mach 12, Kn=0.01 flow of nitrogen about a cylinder: (a) contours of translational temperature obtained with hybrid (MPC), DSMC, and CFD methods; (b) velocity distribution functions in the bow shock.

HYBRID METHOD FOR NONEQUILIBRIUM PLASMA FLOWS

Hall thrusters are an efficient form of plasma electric propulsion for spacecraft. Models have been developed of the plasma plume of such thrusters in order to assess spacecraft integration issues. The high energy ions created by the thruster can sputter spacecraft surfaces upon impact leading to possible damage and subsequent re-deposition. In this section, the plume of a Hall thruster is modeled using a hybrid particle-continuum approach.

Model Description

Hall thrusters primarily use xenon as propellant. The plasma at the exit of a Hall thruster is strongly nonequilibrium with different species possessing different temperatures and velocities. Table 1 lists typical thruster exit conditions for the SPT-100 Hall thruster [10]. In addition, the total number density is of the order of 10^{18} m^{-3} giving a Knudsen number greater than one that places the plasma in the rarefied flow regime. Computational analysis of Hall thruster plumes is regularly performed using a hybrid particle-continuum formulation. The direct simulation Monte Carlo (DSMC) method [3] models the collisions of the heavy particles (ions and atoms). The Particle In Cell (PIC) method [11] models the transport of the ions in electric fields. Overall, a hybrid approach is employed in which the electrons are modeled using a fluid (continuum) description.

Plasma Dynamics

Hall thruster plume models employ a hybrid approach in which heavy species are treated using particles and the electrons are considered as a fluid. Almost all previous hybrid models reduce the electron fluid model to the Boltzmann relation. This requires that the electrons be collisionless, currentless, isothermal, and un-magnetized. All of these assumptions are questionable in a Hall thruster plume, particularly in the plume near-field. Despite the simplicity of the model, these hybrid methods have been quite successful in simulating the far-field properties of a number of different Hall thrusters. As mentioned earlier, the ions and neutrals are treated using a combination of PIC for transporting the ions in electrostatic fields, and DSMC for performing collisions and transporting the neutral atoms.

The most widely used fluid electron approach for plasma plume simulations is the *Boltzmann model*. In this approach, quasi-neutrality is assumed, which allows the ion density to represent the electron density. By further assuming that the electrons are isothermal, collisionless, and un-magnetized, and that their pressure obeys the ideal gas law, $p_e = n_e k T_e$, the Boltzmann relation is obtained from the electron momentum equation:

$$\phi - \phi^* = \frac{kT_e}{e}\ln\left(\frac{n_e}{n_e^*}\right) \qquad (2)$$

where n_e is the electron number density, * indicates a reference state, ϕ is the plasma potential, k is Boltzmann's constant, T_e is the constant electron temperature, and e is the electron charge. The potential is then differentiated spatially to obtain the electric fields.

In the present work, a much more detailed approach is employed that considers all three steady state conservation equations. The electron continuity equation is written as:

$$\nabla^2\psi = n_e n_a C_i \qquad (3)$$

where ψ is a velocity potential and the right hand side is the ionization source term with n_a as the atomic number density, and C_i the ionization rate coefficient. The spatial distribution of the ion particles, treated using DSMC-PIC, gives the electron number density, n_e, under the assumption of charge neutrality. This allows the electron velocity vector to be determined through solution of Eq. (3).

The electron momentum equation is written as a modified Ohm's Law:

$$\bar{j} = \sigma\left[-\nabla\phi + \frac{1}{en_e}\nabla\left(n_e kT_e\right)\right] \qquad (4)$$

where $\bar{j}$ is the current density and σ is the electrical conductivity. Equation (4) is solved for using the charge continuity condition:

$$\nabla.\bar{j} = 0 \qquad (5)$$

to obtain the plasma potential. Finally, the electron energy equation is solved to obtain the electron temperature:

$$\nabla^2 T_e = -\nabla\ln(\kappa_e).\nabla T_e + \frac{1}{\kappa_e}\left(-\bar{j}.\bar{E} + \frac{3}{2}n_e\left(\bar{v}_e.\nabla\right)kT_e + p_e\nabla.\bar{v}_e + 3\frac{m_e}{m_i}\nu_e n_e k\left(T_e - T_H\right) + n_e n_a C_i \varepsilon_i\right) \qquad (6)$$

where κ_e is the electron thermal conductivity, T_H is the heavy species temperature, and $\bar{v}_e$ is the electron velocity.

Collision Dynamics

There are two basic classes of collisions that are important in Hall thruster plumes: (1) elastic (momentum exchange); and (2) charge exchange. Elastic collisions involve only exchange of momentum between the participating particles. For the systems of interest here, this may involve atom-atom or atom-ion collisions. For atom--atom collisions, the Variable Hard Sphere (VHS) [3] collision model is employed.

Charge exchange concerns the transfer of one or more electrons between an atom and an ion. For singly charged ions, the following cross section measured by Miller et al. [12] is used:

$$\sigma_{CEX}\left(Xe, Xe^+\right) = \left(-23.3\log_{10}(g) + 142.2\right)0.8423\times10^{-20}\,\mathrm{m}^2 \qquad (7)$$

Also reported in [9] are charge exchange cross sections for the interaction where a doubly charged ion captures two electrons from an atom. These cross sections are less than a factor of two lower than the values for the singly charged ions at corresponding energies. In the present model, it is assumed that there is no transfer of momentum accompanying the transfer of the electron(s). This assumption is based on the premise that charge exchange interactions are primarily at long range. It is further assumed that atom-ion momentum exchange cross sections are equal to the charge exchange cross section.

Boundary Conditions

For the computation of Hall thruster plumes, boundary conditions must be specified at several locations: (1) at the thruster exit; (2) at the cathode exit; (3) along the outer edges of the computational domain; and (4) along all solid surfaces in the computational domain.

Several macroscopic properties of the plasma exiting the thruster are required for the computations. Specifically, the plasma potential, the electron temperature, and for each of the particle species we require the number density, velocity, and temperature. In the real device, these properties vary radially across the exit plane. The approach to determining these properties involves a mixture of analysis and estimation. The basic performance parameters of mass flow rate, thrust, and total ion current are assumed known. The neutrals are assumed to exit the thrust at the sonic speed corresponding to some assumed value for their temperature. Finally, divergence angles for the lower and upper edges of the exit channel must be assumed. Combining all this information then allows all species densities and the ion velocities to be determined. Determination of the properties of multiple charge states, for example Xe^{2+} is considered in the present study, requires knowledge of the current fraction of that state.

Both fluid and particle boundary conditions are required at the outer edges of the computational domain. The usual field conditions employed simply set the electric fields normal to the boundary edges equal to zero. Similarly the gradients in electron temperature normal to the surfaces of the outer boundaries are set to zero. The particle boundary condition is to simply remove from the computation any particle crossing the domain edge. The results presented in this article consider the thruster to be operating in the vacuum of space. For analysis of thrusters operated in a vacuum chamber, the finite back pressure of the faciliy is included by simulating a fixed density background of xenon atoms at room temperature. These atoms can collide with heavy species emitted by the thruster and so can make an important contribution to the charge exchange plasma. In addition, the background atoms affect the neutral-electron collision frequency that appears in the transport coefficients of the electron fluid model.

The solid wall surfaces of the Hall thruster are also included in the computation. Along these walls, the plasma potential is set to zero and zero gradient in electron temperature is employed. Any ions colliding with the walls are neutralized. Both atoms and neutralized ions are scattered back into the flow field from the surface of the thruster wall assuming diffuse reflection at a temperature of 300 K.

Results

For illustration, we consider the plumes generated by SPT-100 Hall thrusters employed on the Russian Express spacecraft. A variety of sensors were employed on board the two spacecraft to characterize the effects of firing the Hall thrusters on the spacecraft operation and environment. The present study focuses on measurements of ion energy distributions. The analysis presented briefly here is described in more detail by Boyd [10]. The operating conditions of the SPT-100 Hall thruster considered in the present study are as follows: flow rate = 5.3 mg/s, discharge current = 4.5 A (82% is attributed to ions of which 30% by current fraction is attributed to Xe^{2+}), discharge voltage = 300 V, specific impulse = 1,600 sec. The computational domain extends more than 10 m axially from the thruster exit and 10 m radially from the thruster centerline to cover all of the Express probe locations. This is achieved using a mesh containing 190 by 175 non-uniform, rectangular cells. The radial mesh spacing at the thruster exit is 5 mm giving just 4 cells across the exit of the thruster. In a typical computation approximately 4 million particles are employed with about 60% representing ions (both single and double charged). The neutral atom flow is first allowed to reach a steady state by using a large time step. The ions are then subsequently introduced with a time step of about 10^{-7}s. The computations reach a steady state for the ions after about 15,000 iterations and solutions are then averaged over a further 10,000 iterations. The total computation time is about 24 hours on a personal computer.

In Figs. 3(a) and 3(b), contours are shown of the plasma and neutral atom number densities, respectively. These show that the two populations follow quite different plume expansion dynamics. The bubble of charge exchange plasma formed vertically above the thruster exit plane can be seen clearly in Fig. 3(a).

The ion energy distribution measured on Express in the primary beam near to the centerline (at 7 deg.) and a distance of 3.76 m is considered in Fig. 4(a), where the Express data is compared with the results of the simulation. Note, in terms of plotting style, that exact agreement between the data sets would mean that the solid line employed for the model results would go through the center of the horizontal bar of each column of the histogram used for the Express data. The data measured in space provides a narrower distribution than profiles measured in ground facilities and this is perhaps explained by collisional broadening present in the vacuum tank experiments. In Fig. 4(a), there is clearly very good agreement between the simulation and the Express data.

The ion energy distribution obtained on Express at the large angle of 77 deg and a distance of 1.40 m is now considered. This location is of particular interest since it is characterized primarily by charge exchange ions. Very few beam ions are expected to exit the Hall thruster at such large angles. In Fig. 4(b), the Express data are compared with the results from the simulation. Figure 4(b) includes a high energy structure measured on-board the Express spacecraft that extends up to values associated with primary beam ions of about 260 eV. These high energies are not simulated by the model, although the peak of the distribution at about 28 eV is very well predicted.

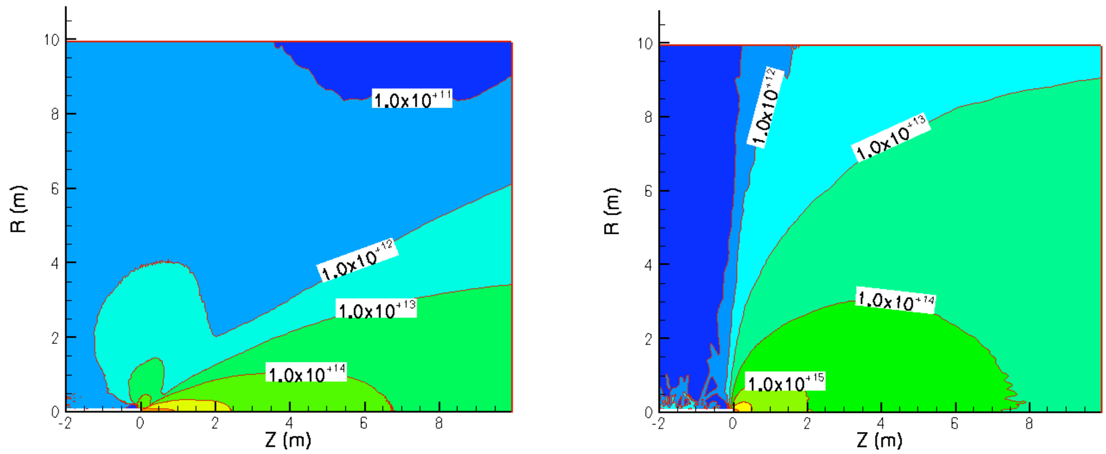

FIGURE 3. Plume results for the SPT-100 Hall thruster: (a) Xe^{+} number density; (b) Xe number density.

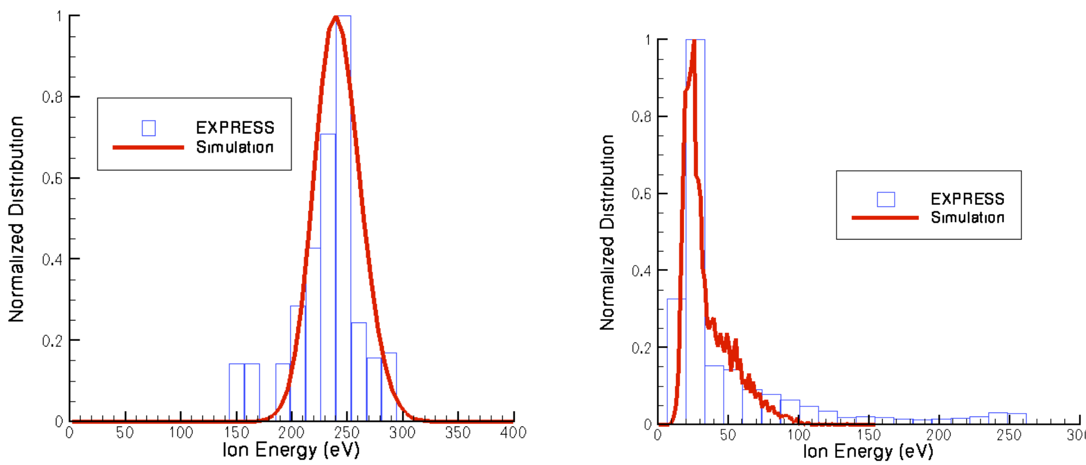

FIGURE 4. Ion energy distribution functions in the plume of a Hall thruster: (a) main beam; (b) charge exchange plasma.

Table 1: Plasma properties at the exit of the SPT-100 Hall thruster.

Property/Species	**Xe**	**Xe+**	**Xe2+**	**E-**
Number Density (m^{-3})	1.2×10^{18}	2.4×10^{17}	2.6×10^{16}	2.9×10^{17}
Temperature	750 K	1 eV	1 eV	6 eV
Velocity	280 m/s	18 km/s	25 km/s	-6 km/s

An example of use of the hybrid method to analyze a Hall thruster experiment performed in a vacuum facility is shown in Fig. 5. In this case, a high power thruster operated at 10 kW is in the 12V vacuum chamber is considered [13]. Complex geometric structures representing baffles and pumping surfaces inside the chamber are included the analysis. Future directions in the development of this technique include extension to 3D, inclusion of magnetic field effects, and improved consideration of the thruster cathode.

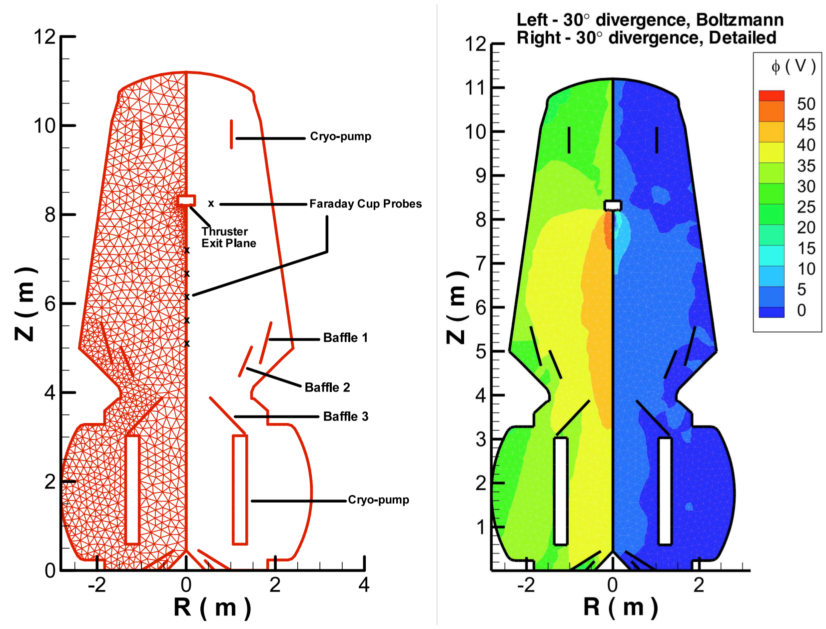

FIGURE 5. Hybrid analysis of a 10 kW Hall thruster operated in a vacuum chamber [13]: (a) mesh; (b) plasma potential.

SUMMARY

Numerical simulation of nonequilibrium gas and plasma dynamics represents a multi-scale problem that can be addressed with physical accuracy and numerical efficiency using hybrid particle-continuum techniques. For hypersonic gas dynamics, a hybrid method was described that decomposes a flow domain into regions that are simulated using continuum (CFD) or particle (DSMC) methods. This technique is able to reproduce results from full DSMC computations at the level of the velocity distribution function while requiring only a fraction of the cost. For plasma jets, a hybrid method was described that uses a particle method (DSMC-PIC) for the heavy species, and a fluid approach for the electrons. This technique makes it possible to conduct two-dimensional simulations in just a few hours that offer excellent agreement with data measured during space operation.

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Hybrid Particle-Continuum Methods For Nonequilibrium Gas and Plasma Flows

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Overview

- Nonequilibrium gas and plasma dynamics
- Modeling of hypersonic aerothermodynamics:
  - hybrid fluid-particle method
  - illustrative examples
- Modeling of spacecraft plasma propulsion systems:
  - effects of thruster plumes
  - hybrid fluid-particle method
  - example: Hall thruster plumes

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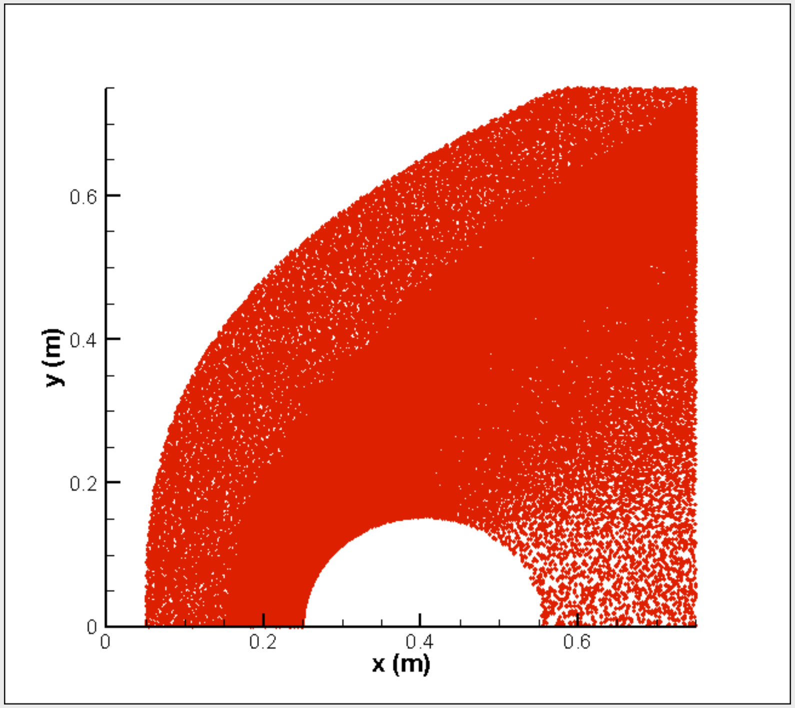
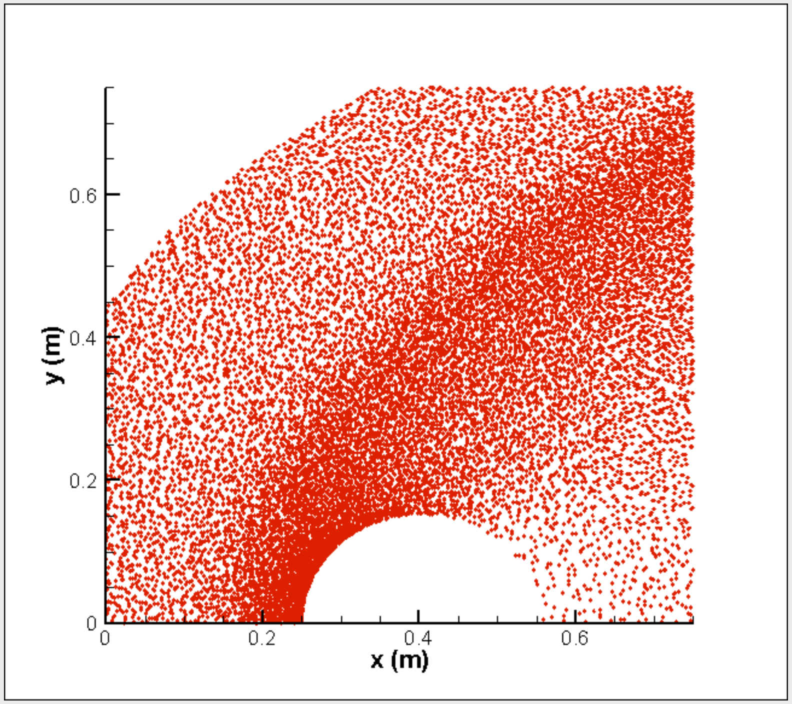
What is Nonequilibrium?





Continuum flow regime:
- small Kn=λ/L
- high density and/or large L
- many collisions
- thermodynamic equilibrium

Rarefied flow regime:
- large Kn=λ/L
- low density and/or small L
- few collisions
- nonequilibrium

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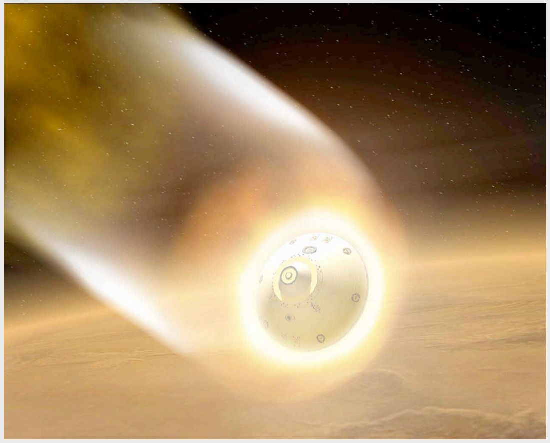
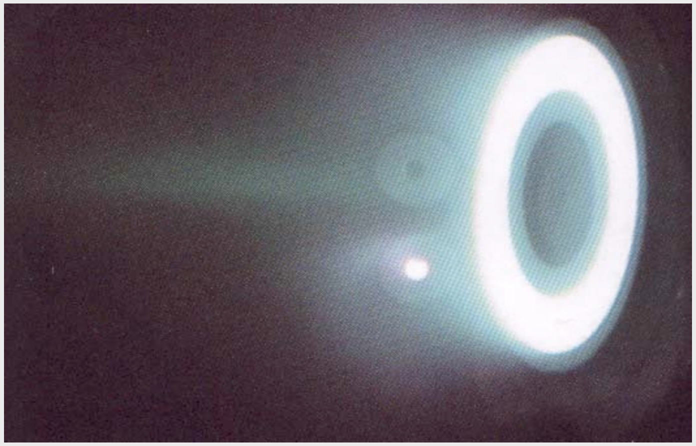
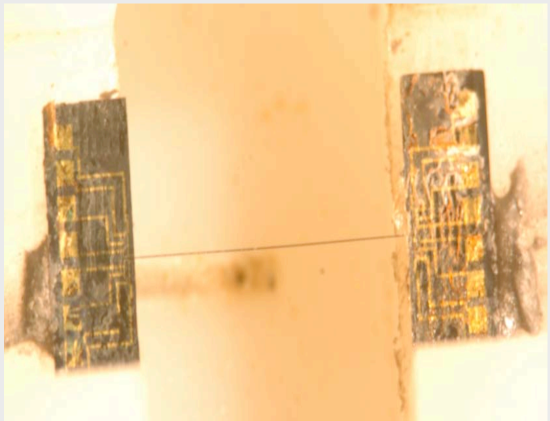
Nonequilibrium Systems



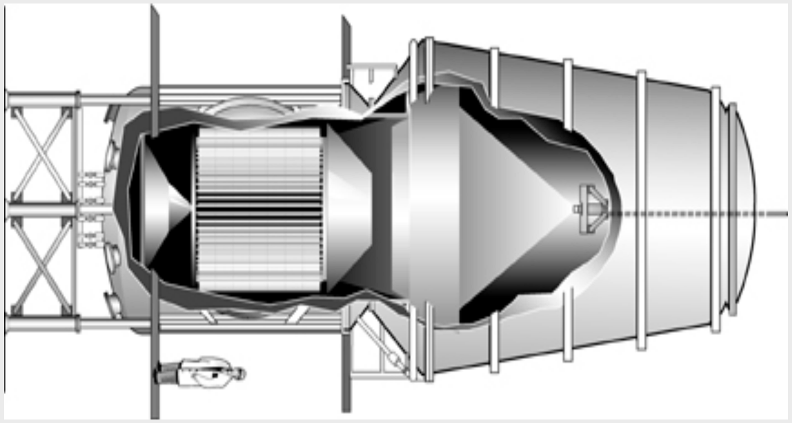
Hypersonic Vehicles



Spacecraft Propulsion



Micro-scale Gas Flows



Vacuum Systems

Distribution A: Approved for public release; distribution unlimited.

Computation of Nonequilibrium Gas Flow

Flow Regimes:

continuum | slip | transitional | free-molecular

Kn 0.01 0.1 1

Model Accuracy:

DSMC

Boltzmann Equation

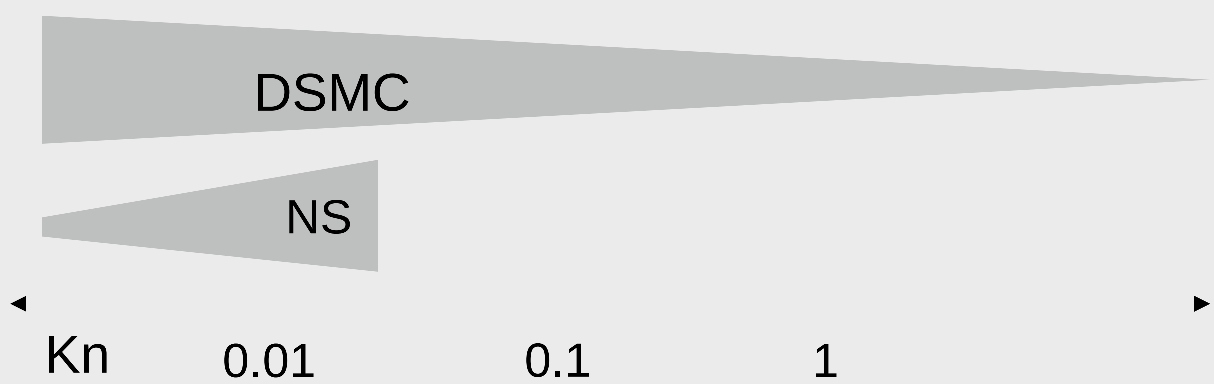
Collisionless Boltzmann Eqn

N-S

Euler

Burnett

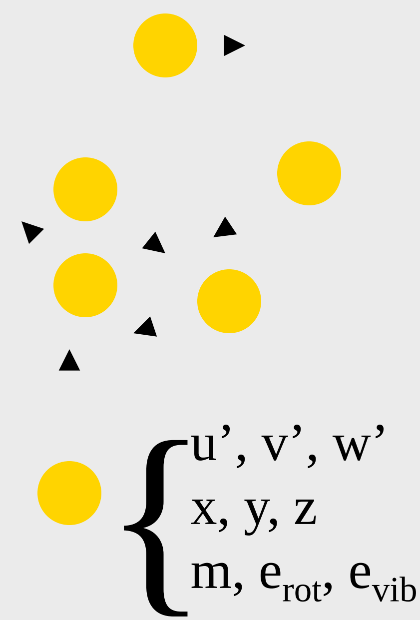
Numerical Cost:



Distribution A: Approved for public release; distribution unlimited.

Direct Simulation Monte Carlo Method (DSMC)

- Particle method for nonequilibrium gas flows:
  - developed by Bird (1960's)
  - particles move/collide in physical space
  - particles possess molecular level properties, e.g. u' (thermal velocity)
  - cell size $\Delta x \sim \lambda$, time step $\Delta t \sim \tau$
  - collisions handled statistically (not MD)
  - internal energy relaxation, chemistry
  - gas-surface interactions



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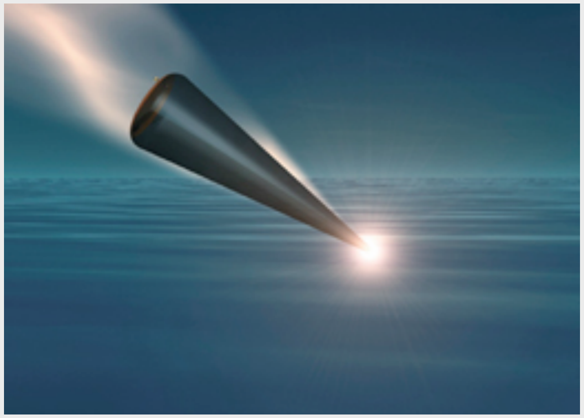
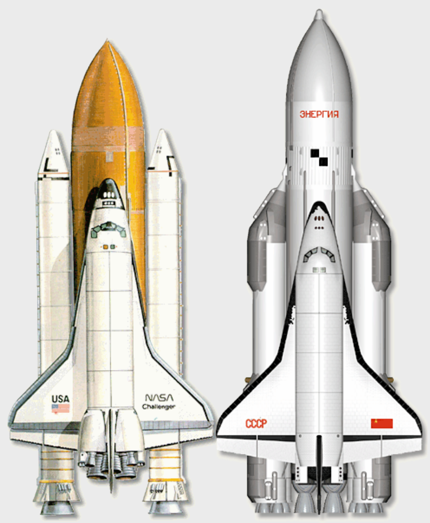
Hypersonic Vehicles: Ma > 5



Ballistic Missiles

Entry Capsules



Space Planes

Air-Breathing Cruisers

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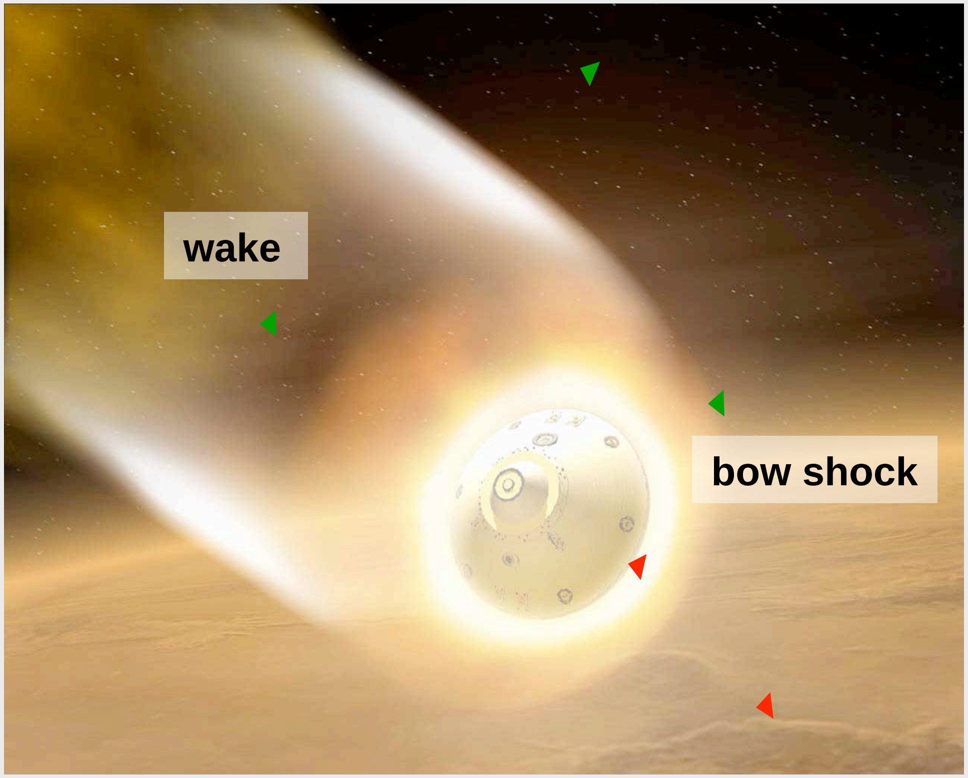
Hybrid Method for Hypersonic Flows

- Hypersonic vehicles encounter a variety of flow regimes:
  - continuum: modeled accurately and efficiently with CFD
  - rarefied: modeled accurately and efficiently with DSMC



Rarefied DSMC approach:
- based on kinetic theory
- high altitude, low density
- small length scales

Continuum CFD approach:
- solve NS equations
- low altitude
- long length scales

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Hybrid CFD-DSMC Approach

Scalabrin and Boyd
AIAA-2006-3773

Dietrich and Boyd
J. Comp. Phys., **126**, 1996

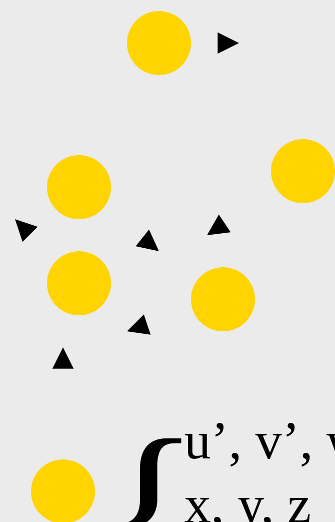
NS solver (LeMANS) ◂ ▸ interface ◂ ▸ DSMC (MONACO)

NS solver (LeMANS)

- 2D/3D unstructured mesh
- Modified Steger-Warming flux-vector splitting, parallel
- Point-implicit time integration
- Many physical models

DSMC (MONACO)

- 2D/3D unstructured mesh
- Parallel, domain decomposition
- Many physical models



$$\rho_i,\ T_t,\ T_r,\ T_v$$
$$u,\ v,\ w$$

$$\left\{\begin{array}{l} u',\ v',\ w' \\ x,\ y,\ z \\ m,\ e_{rot},\ e_{vib} \end{array}\right.$$

Distribution A: Approved for public release; distribution unlimited.

Simulation Codes

- CFD=LeMANS code:
  - developed by Scalabrin & Boyd (2006)
  - solves the Navier-Stokes equations
  - isothermal, no-slip wall conditions employed
  - transport coefficients from collision integrals
- DSMC=MONACO implementation:
  - developed by Boyd et al. since 1996
  - general 2D/AXI/3D, parallel, unstructured meshes
  - isothermal wall, some slip always present
  - collision model consistent with CFD transport

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Continuum Breakdown

- How do we know when CFD fails?
  - continuum breakdown parameter
  - gradient-length Knudsen number, Kn_{GL}

$$Kn_{GL-Q} = \frac{\lambda}{Q}\left|\nabla Q\right|$$

$$Kn_{GL} = \max(Kn_{GL-\rho}, Kn_{GL-V}, Kn_{GL-T})$$

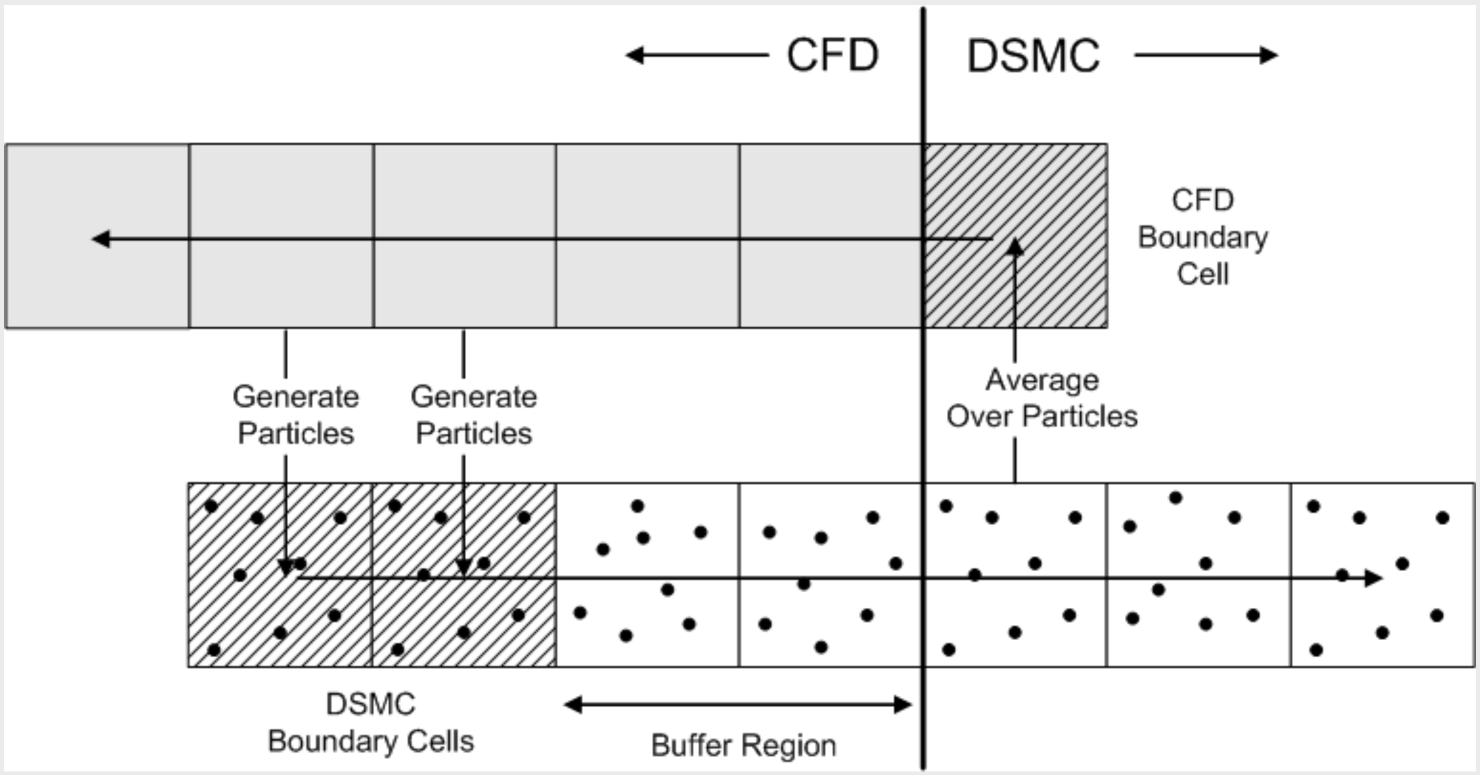
- For regions in the flow field where $Kn_{GL} < 0.05$
  - it has been shown that

$$\left|\frac{DSMC_{SOL'N} - CFD_{SOL'N}}{DSMC_{SOL'N}}\right| < 5\%$$

Distribution A: Approved for public release; distribution unlimited.

Hybrid Coupling Method

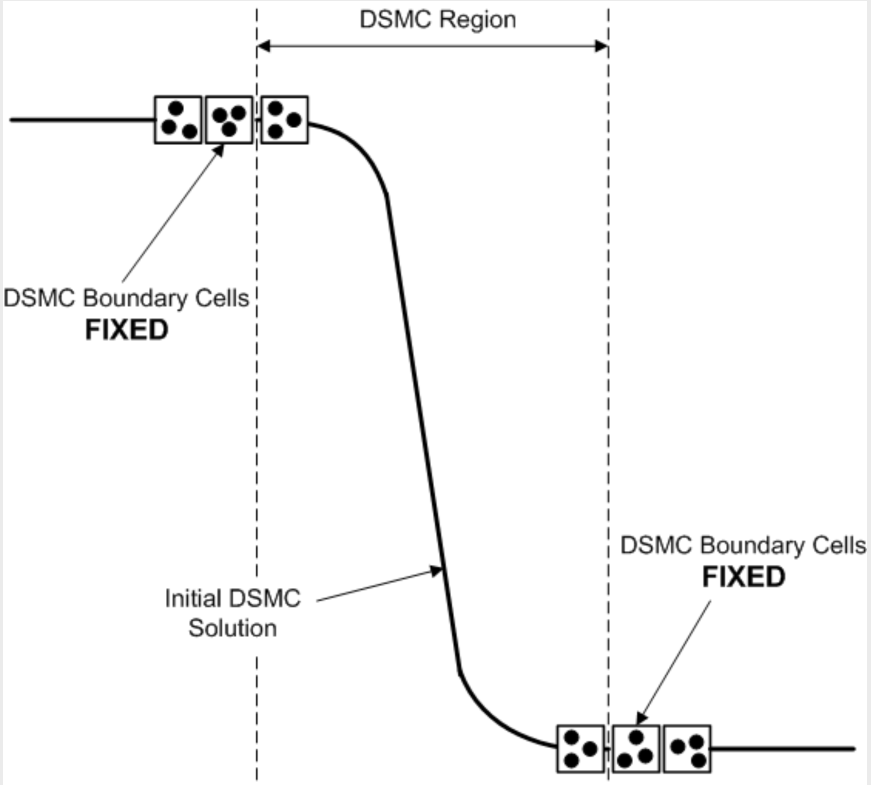
- State-based coupling
  - Use existing CFD and DSMC boundary procedures



Distribution A: Approved for public release; distribution unlimited.

DSMC Boundary Conditions

- Generate particles in the interior and boundary of DSMC domain
- Use the Chapman-Enskog distribution based on local CFD information



Velocity profile through a normal shock

Distribution A: Approved for public release; distribution unlimited.

CFD Boundary Conditions

- Average DSMC data communicated to CFD has huge fluctuations

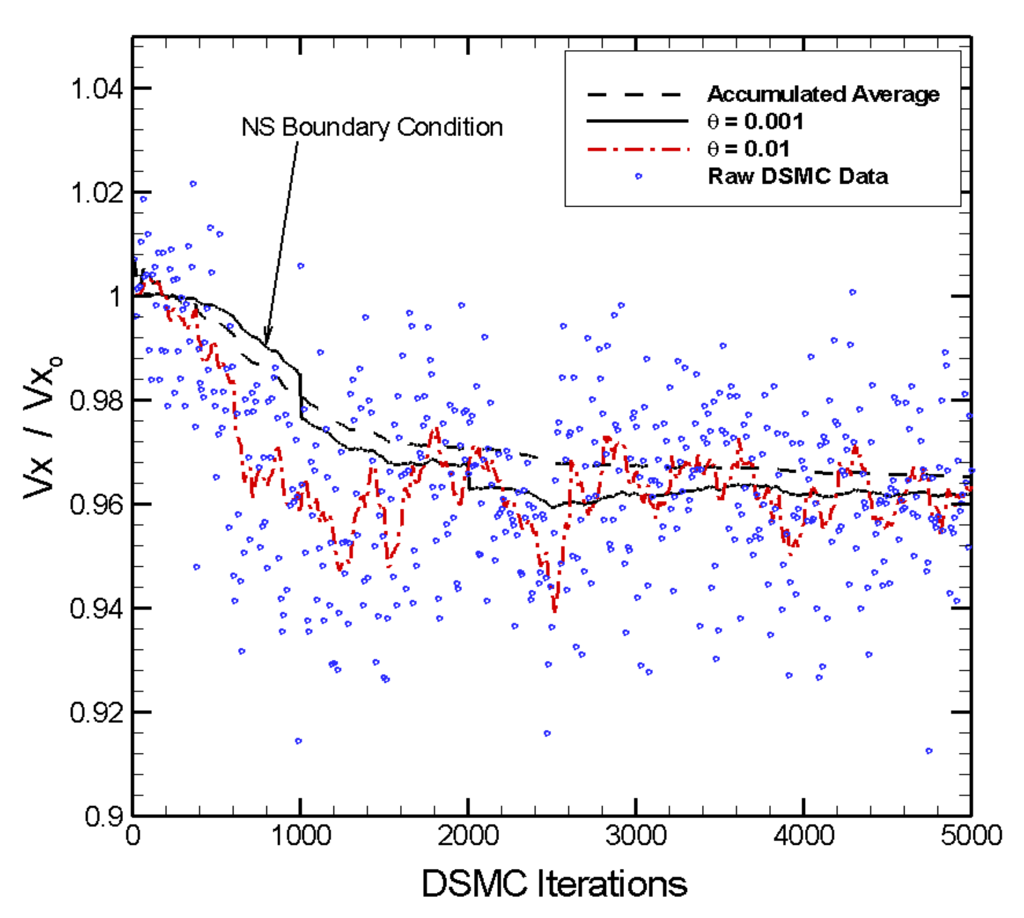
- Sub-relaxation technique (Sun and Boyd, 2005)

$$\overline{A_j} = (1-\theta)\overline{A_{j-1}} + \theta A_j$$

- History before time-step i is removed by

$$\overline{A_j}' = \overline{A_j} + \frac{(1-\theta)^{j-i}}{1-(1-\theta)^{j-i}}(\overline{A_j} - \overline{A_i}'),$$

$$j = \tfrac{1}{\theta} + i$$



Distribution A: Approved for public release; distribution unlimited.

Hybrid CFD-DSMC Algorithm

Initial CFD solution
Decompose DSMC and CFD regions
Generate particles in DSMC regions

Iterate DSMC regions
Use sub-relax avg. to track macro changes

Apply Kn_{GL} to update interface locations

Update CFD BCs and converge

No

Have interfaces stopped moving?

Yes

Lock interfaces
Sample DSMC
Converge CFD

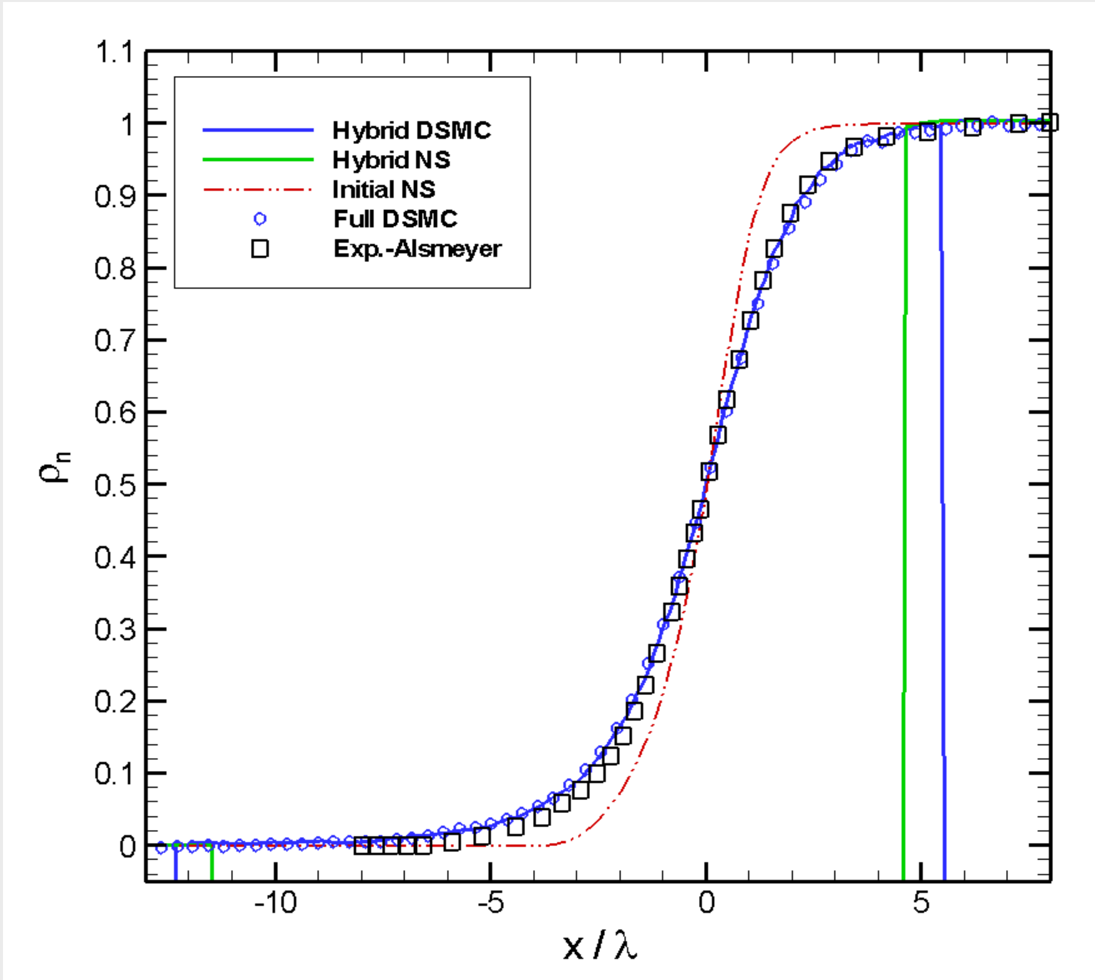
Distribution A: Approved for public release; distribution unlimited.

Example: Normal Shock Waves

- Argon and nitrogen normal shocks investigated:
  - relatively simple hypersonic flow
  - Alsmeyer experimental measurements
  - well-known case for testing new algorithms
- Simulations:
  - modeled in 2D (400 x 5 cells)
  - initialized by jump conditions
  - pure DSMC
  - pure CFD (Navier-Stokes equations)
  - hybrid code initialized by CFD solution

Distribution A: Approved for public release; distribution unlimited.

Argon Shock Wave: Mach 9



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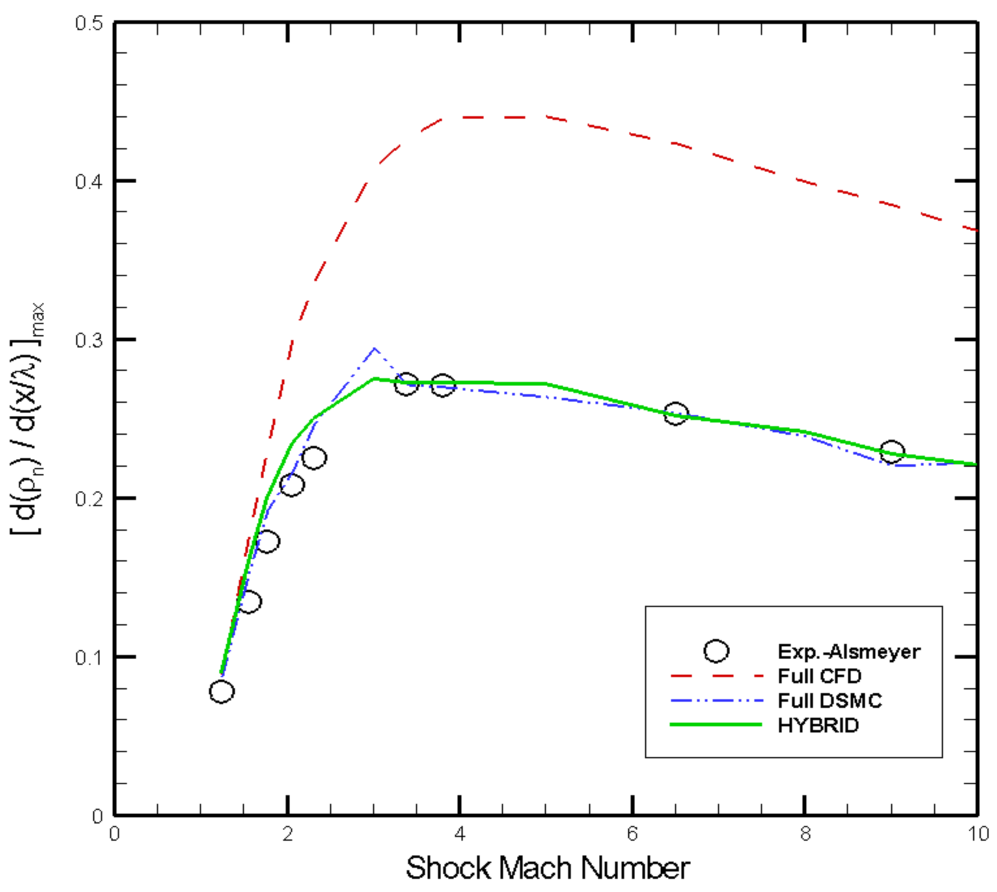
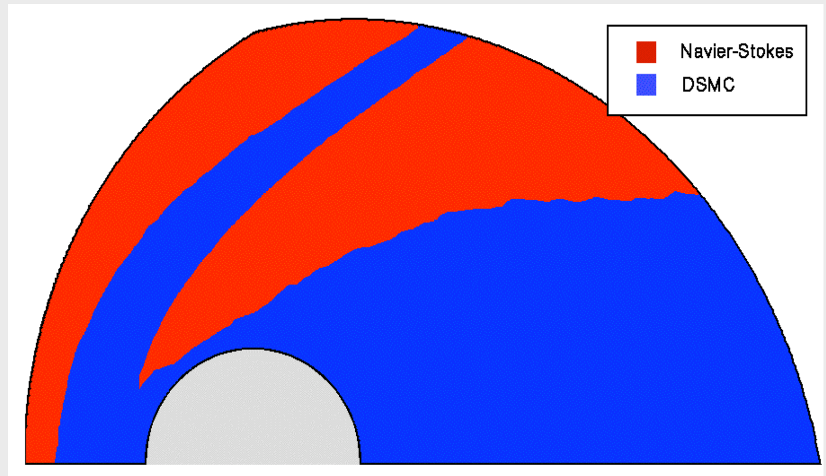
Physical Accuracy

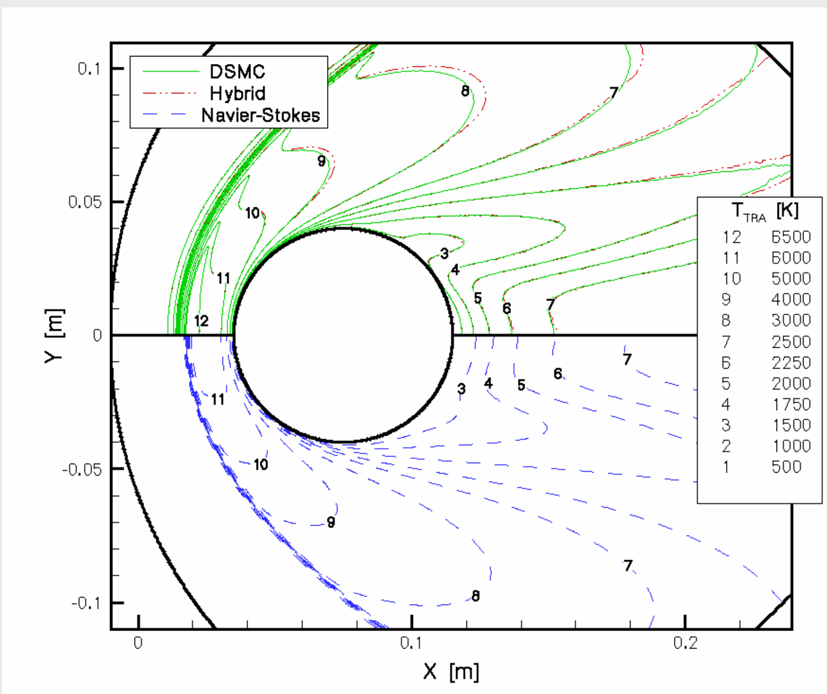


Distribution A: Approved for public release; distribution unlimited.

2D Cylinder Flow of N_2: Ma=12, Kn_∞=0.01

- CFD corrections needed in:
  - bow shock
  - boundary layer
  - wake



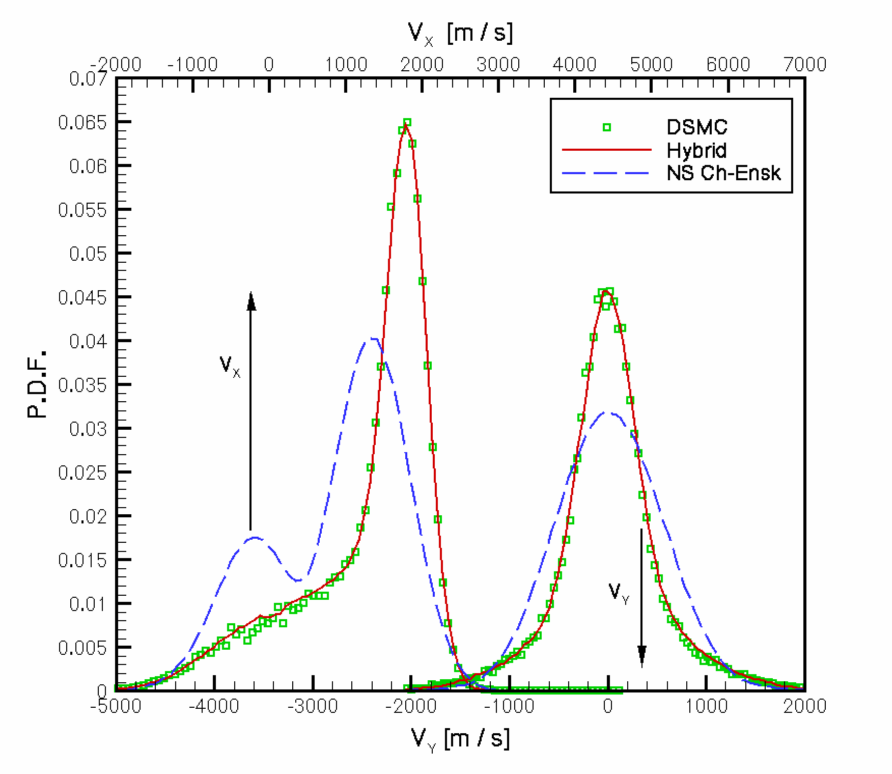


- Hybrid algorithm:
  - initialized by CFD
  - final solution agrees with pure DSMC

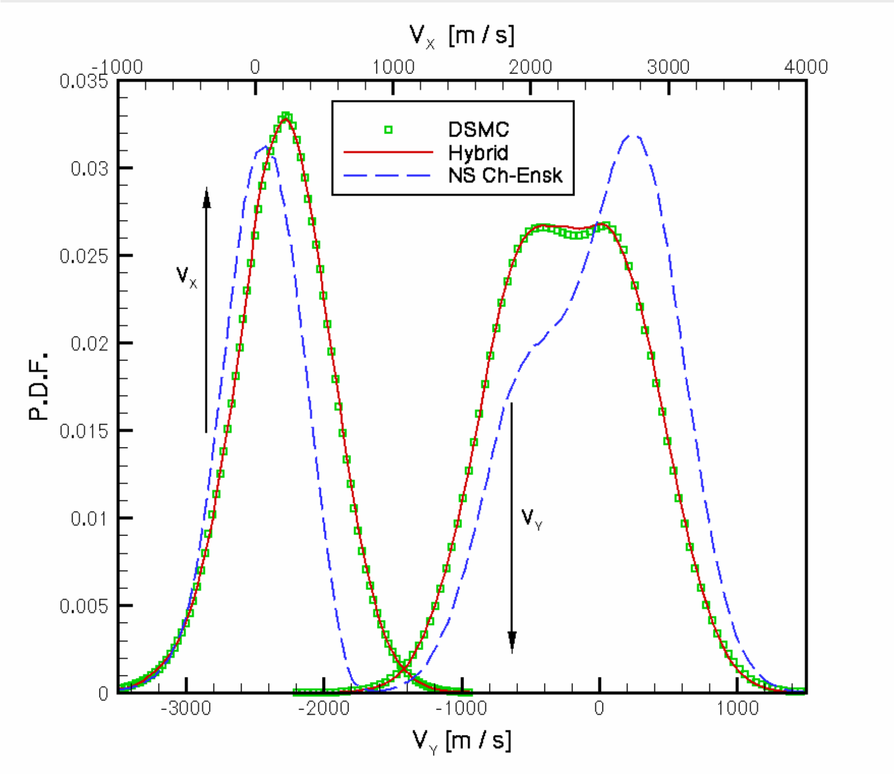
Distribution A: Approved for public release; distribution unlimited.

Local Velocity Distributions

- Hybrid method is physically accurate to the level of the particle velocity distribution



Mid-shock along stagnation line



135º around cylinder surface

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Future Directions for Hypersonic Hybrid Method

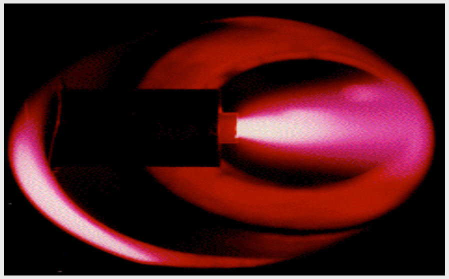
- Algorithm development:
  - generalized mesh, 3D, parallel (Deschenes)
  - DSMC: implicit and/or other acceleration schemes
  - other approaches: e.g. LD-DSMC (Burt)
- Physics development:
  - chemically reacting gas mixture
  - extension to plasma flows (MHD)
- Development of hybrid methodology:
  - refinement of breakdown parameters
  - evaluation against data (measured, computed)

Distribution A: Approved for public release; distribution unlimited.

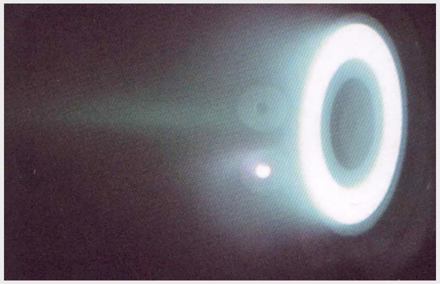
Spacecraft
Plasma Propulsion Systems

Tasks: orbit transfer and maintenance

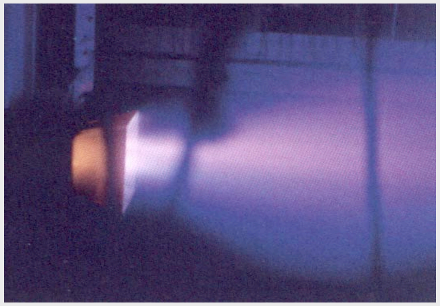
Electrothermal Propulsion
Resistojet thrusters
Arcjet thrusters



Electrostatic Propulsion
Ion thrusters
Hall thrusters

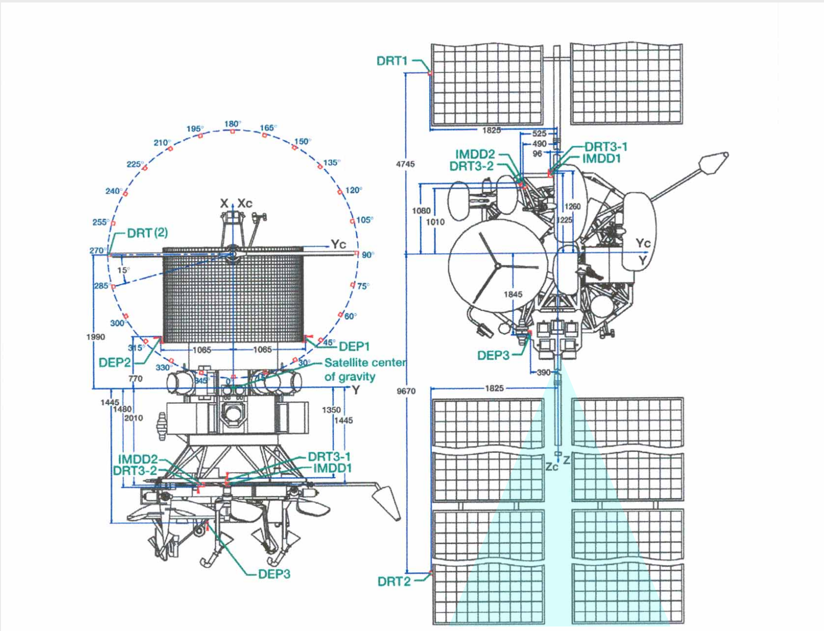


Electromagnetic Propulsion
Pulsed plasma thrusters
Magnetoplasmadynamic thrusters



Distribution A: Approved for public release; distribution unlimited.

Spacecraft Integration: Effects of Thruster Plumes



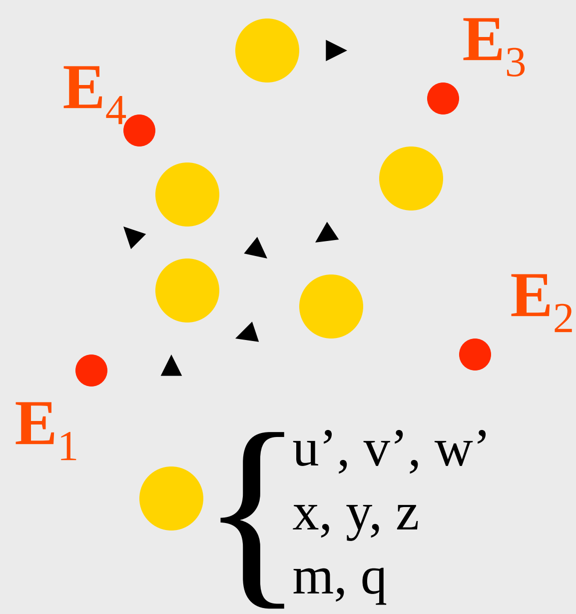
- Spacecraft-plume interaction:
  - ions diverge from thruster
  - energetic impingement
  - material sputtering
  - subsequent re-deposition
  - reduced functionality
- Accurate simulations:
  - experiments difficult
  - Kn~1 at thruster exit
  - charge exchange
  - electro-static forces

Distribution A: Approved for public release; distribution unlimited.

Plume Plasma Dynamics: Particle In Cell (PIC)

- *Hybrid method*: *particles* for ions/atoms (nonequilibrium)
  fluid for electrons due to small mass

- Heavy species treated using PIC:
  - weight-to-mesh (Ruyten, 1993)
  - charge neutrality => n_e
  - ϕ from **fluid electron** models
  - differentiate ϕ for electric fields, **E**
  - weight-to-particles to accelerate
  - neutral transport included
  - combined with DSMC for collisions



Distribution A: Approved for public release; distribution unlimited.

Plume Electron Dynamics: 1. Boltzmann Relation

- Standard approach for plasma thruster plumes :
  - derived from electron momentum equation
  - currentless, isothermal, un-magnetized, collisionless
  - charge neutrality provides potential from ion density:

$$\phi - \phi^* = \frac{kT}{e} \ln\left(\frac{n}{n^*}\right)$$

  - n^*, ϕ^* are reference values

- Required models/inputs:
  - boundary conditions at thruster exit

Distribution A: Approved for public release; distribution unlimited.

Plume Electron Dynamics: 2. Detailed Fluid Model

- ADI solution of steady-state conservation equations:
  - electron continuity equation (including ionization)

$$\nabla^2\psi = n n_a C_i \text{ where } \nabla\psi = n\bar{u}$$

  - generalized Ohm's law (electron momentum equation)

$$\nabla.\bar{j} = 0 \text{ where } \bar{j} = \sigma\left[-\nabla\phi + \frac{1}{en}\nabla(nkT)\right]$$

  - electron energy equation (including ionization)

$$\nabla^2 T = -\nabla\ln(\kappa).\nabla T + \frac{1}{\kappa}\left(-\bar{j}.\bar{E} + \frac{3}{2}n(\bar{u}.\nabla)kT + p\nabla.\bar{u} + n n_a C_i \varepsilon_i\right)$$

- Required models/inputs:
  - transport/ionization coefficients for propellant system
  - boundary conditions at thruster and cathode exits

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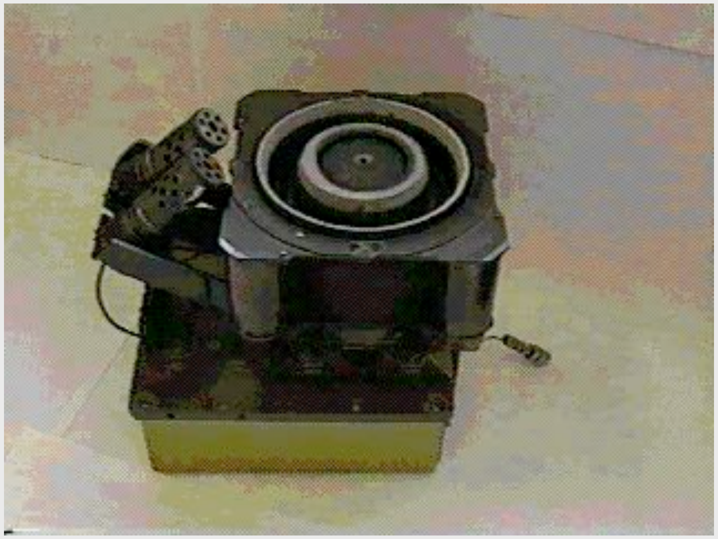
Thruster Exit Conditions

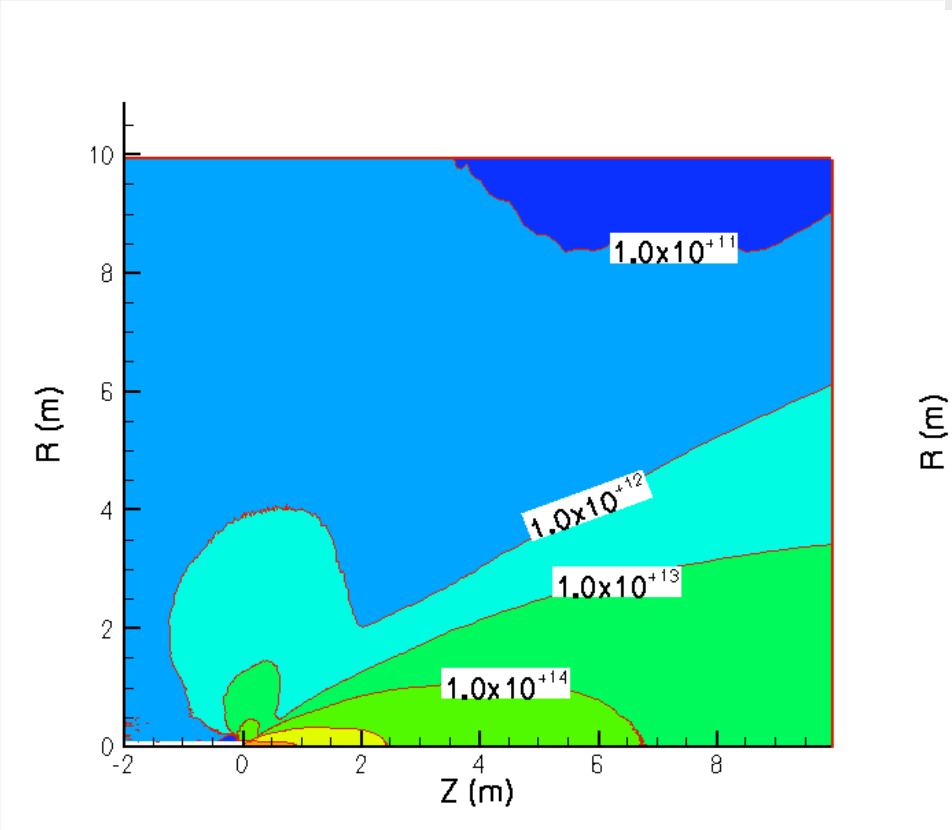
For the SPT-100



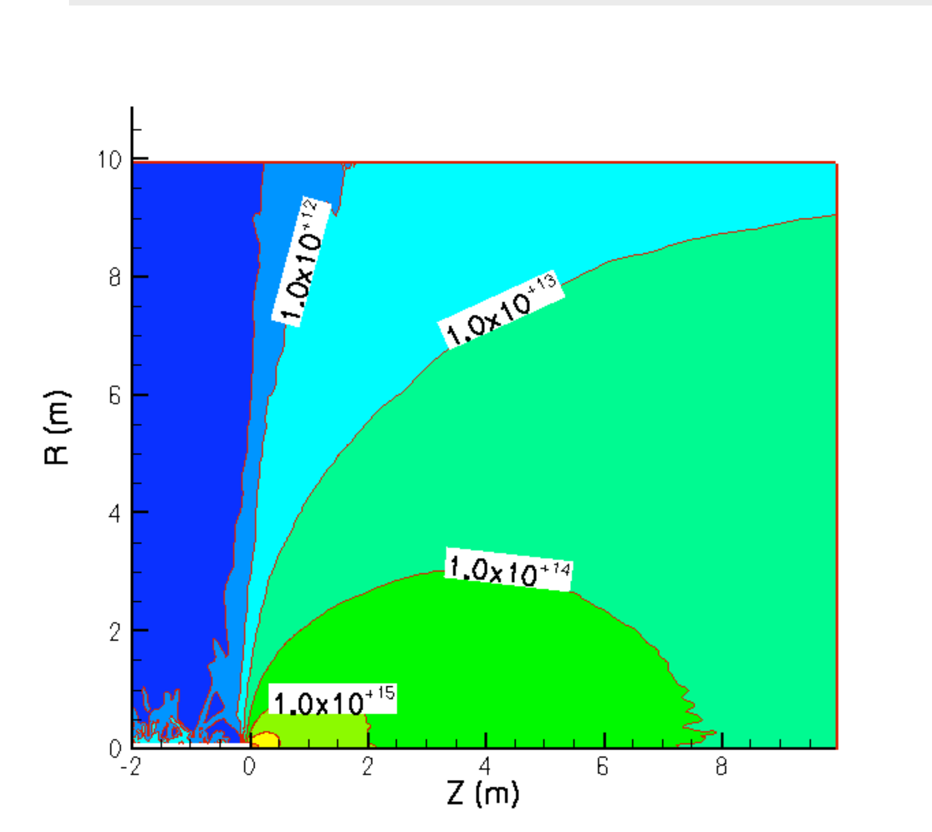
Inner Diameter	60 mm
Outer Diameter	100 mm
Plasma Density	$2.4\text{x}10^{17}\ \text{m}^{-3}$
Neutral Density	$2.0\text{x}10^{18}\ \text{m}^{-3}$
Ion Velocity	18.5 km/s
Neutral Velocity	280 m/s
Electron Temperature	6 eV
Ion Temperature	1 eV
Neutral Temperature	750 K

Distribution A: Approved for public release; distribution unlimited.

Flow Field:
Heavy Particle Properties



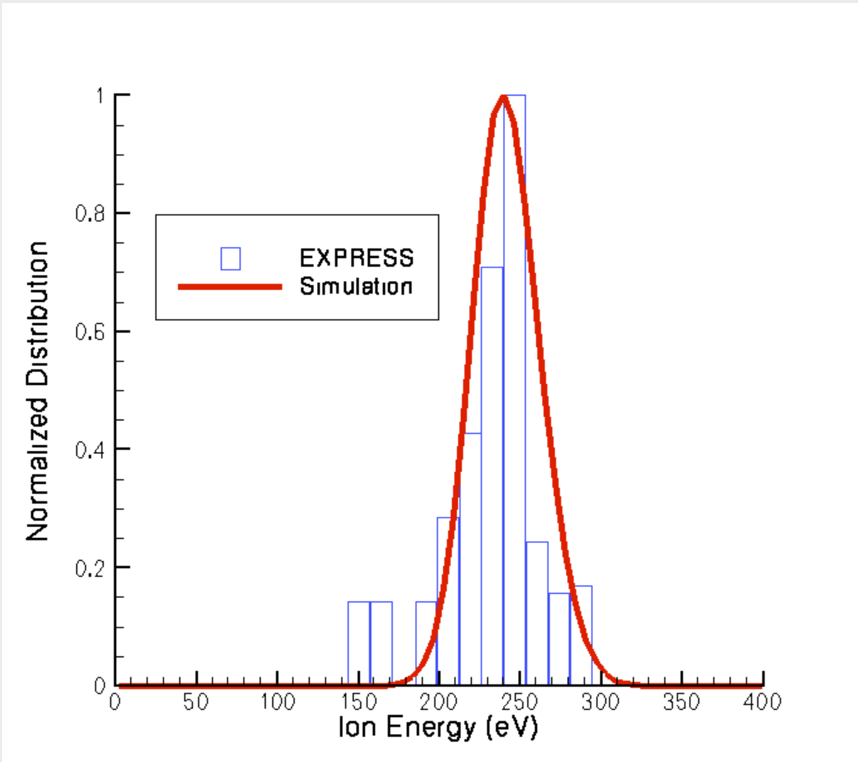
Ion Number Density (m^{-3})

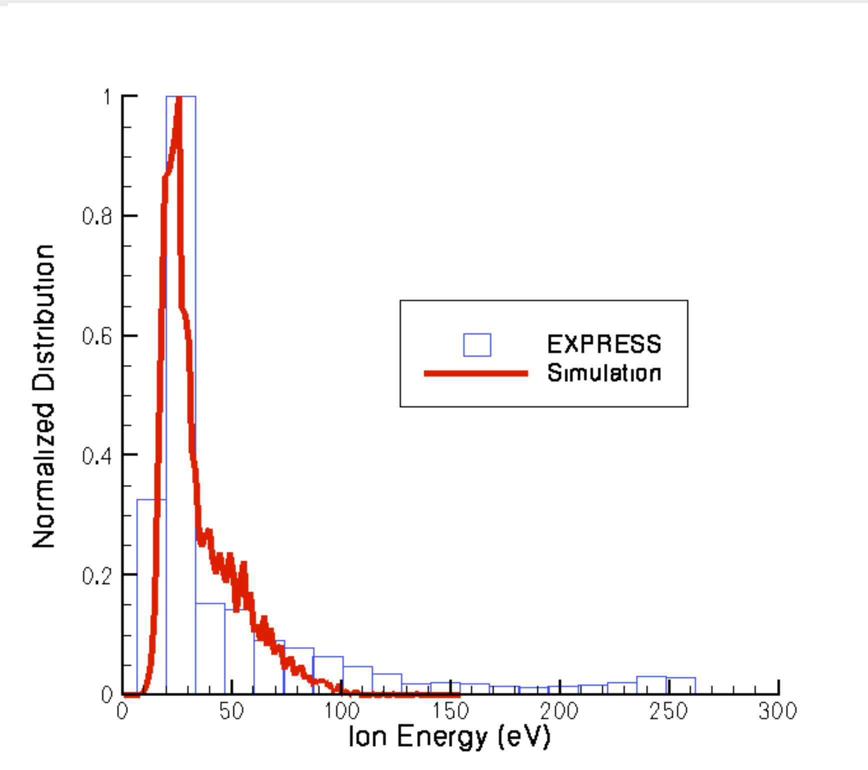


Atom Number Density (m^{-3})

Distribution A: Approved for public release; distribution unlimited.

Ion Energy Distributions





Primary Beam
(z=4 m, θ=7.5 deg.)

CEX Plasma
(z=1.4 m, θ=77.5 deg.)

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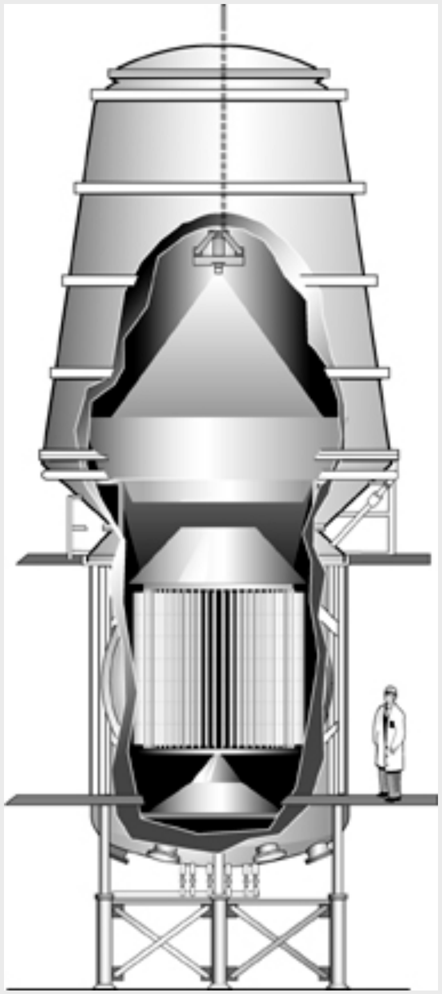
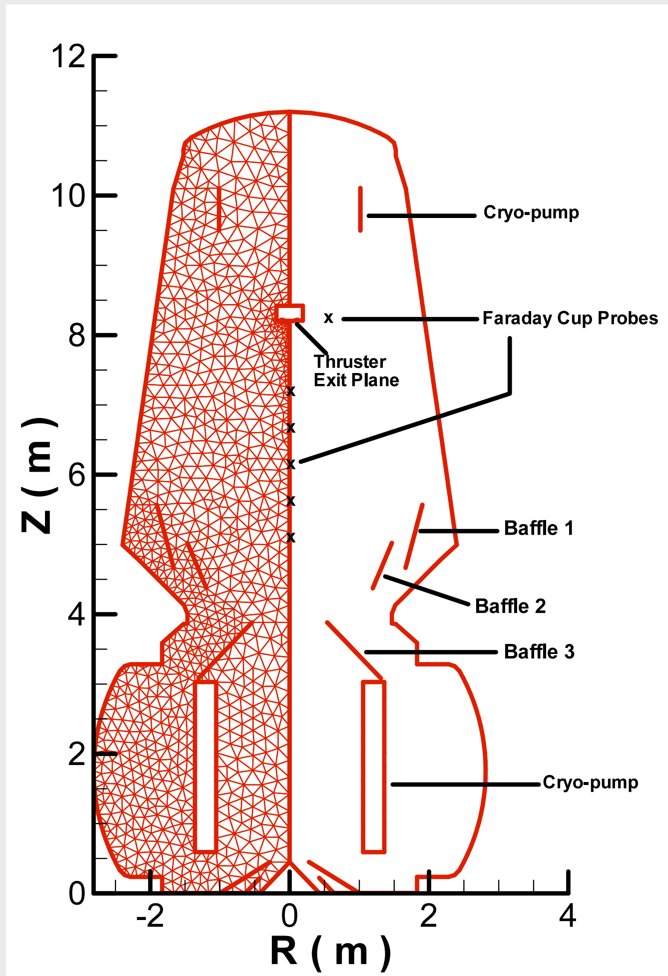
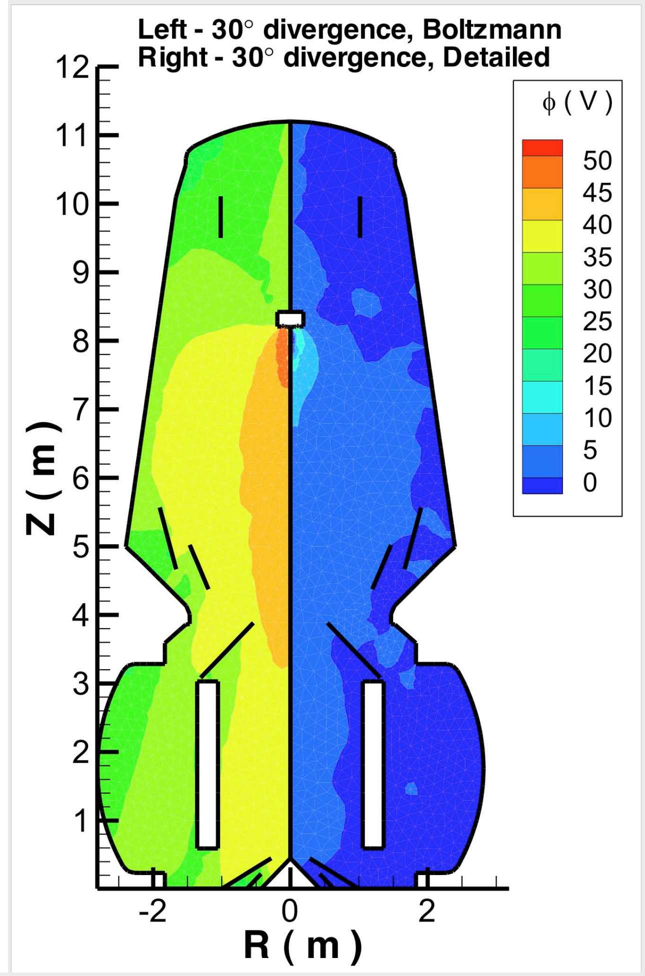
Analysis of The 12V EP Test Facility







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Future Directions for Hybrid Plume Modeling

- Improved numerical algorithms:
  - unstructured 3D meshes
- Improved physical modeling:
  - plasma transport coefficients
  - thruster exit conditions from thruster simulation
  - effects on electrons of thruster magnetic field
- Further assessments of the models:
  - other Hall thrusters (e.g. anode layer thrusters)
  - other EP thrusters (e.g. MPD, ion, PPT)

Distribution A: Approved for public release; distribution unlimited.

Summary

- Hybrid method for hypersonic aerothermodynamics:
  – combine accuracy of DSMC, efficiency of CFD
  – decompose domain into CFD and DSMC regions
  – hybrid algorithm successfully “corrects” CFD
  – best case (so far) more than 30 times faster than DSMC

- Hybrid method for spacecraft thruster plumes:
  – impossible to model electrons as particles (mass)
  – particles for ion/atoms, fluid for electrons
  – both approaches used simultaneously everywhere
  – good agreement with plume measurements

Distribution A: Approved for public release; distribution unlimited.